=> d his

(FILE 'HOME' ENTERED AT 18:39:14 ON 27 OCT 2003)

FILE 'MEDLINE, CAPLUS, BIOSIS, EMBASE, SCISEARCH, AGRICOLA' ENTERED AT
18:39:49 ON 27 OCT 2003
L1 8793047 S DRUG
L2 336024 S L1 (P) (DELIVER? OR TARGET?)
L3 30675 S ANCHORING
L4 1701425 S LINK?
L5 69 S L1 (P) L3 (P) L4
L6 173443 S (ION CHANNEL) OR (MEMBRANE RECEPTOR)
L7 313089 S (CALCIUM OR SODIUM OR POTASSIUM) (W) CHANNEL
L8 113603 S (BETA ADRENERGIC RECEPTOR) OR (MEMBRANE TRANSPORTER)
L9 543761 S L6 OR L7 OR L8
L10 0 S L5 (P) L9
L11 36 S L2 (P) L3 (P) L4
L12 0 S L11 (P) L9
L13 208044 S (LOCAL ANESTHETIC) OR BENZOCAINE OR LIDOCAINE OR DIBUCAINE OR
L14 261404 S BENZODIAZEPINE OR HYDANTOIN OR SIOPRENOID OR THIAZOLIDINONE O
L15 178290 S ANTINEOPLASTIC AGENT
L16 640970 S L13 OR L14 OR L15
L17 15 S L16 (P) L3 (P) L4
L18 0 S L17 (P) L9
L19 70933 S (SULFHYDRYL REACTIVE) OR ALKYLATING OR ACYLATING
L20 216916 S METHANTHIOSULFONYL OR DITHIOPYRIDYL OR DISULFIDE OR (HALO KET
L21 1510 S L1 (P) (L19 OR L20) (P) L4
L22 13 S L21 (P) L9
L23 7 DUPLICATE REMOVE L22 (6 DUPLICATES REMOVED)
L24 1 S L23 (P) (TARGET? OR DELIVER?)
L25 764445 S (BINDING SITE) OR (SITE SPECIFIC)
L26 1 S L25 AND L23
L27 19 S BACKX PETER/AU
L28 6 S DIME DAVID/AU
L29 1 S KIMMELDIRK KLAUS/AU
L30 1 S (L27 OR L28 OR L29) AND L2

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	Type	L #	Hits	Search Text	DBs	Time Stamp	Comments	Error Definition	Errors
1	BRS	L1	251291	drug	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:04			0
2	BRS	L2	999	anchoring adj (group or moiety or compound or agent)	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:05			0
3	BRS	L3	54713	linking adj (group or agent or compound)	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:06			0
4	BRS	L4	47550	linker	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:06			0
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6	BRS	L6	3	1 same 2 same 5	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:10			0
7	BRS	L7	7373	ion adj channel	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:11			0
8	BRS	L8	4222	membrane adj receptor	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:11			0
9	BRS	L9	0	6 same (7 or 8)	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:12			0
10	BRS	L10	18638	(local adj anesthetic) or benzocaine or lidocaine or dibucaine or chlorpromazine	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:12			0

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11	BRS	L12	366985	benzodiazepine or hydantoin or isoprenoid or thiazolidinone or metathiazanone or pyrrolidine or morpholino or (cycloadj carboxylic adj acid) or phenyalkylamine or dihydropyridine	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/10/27 18:16			0
12	BRS	L13	4212	antineoplastic adj agent	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:16			0
13	BRS	L14	7721	12 same 1	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:17			0
14	BRS	L15	0	(10 or 13 or 14) same 2 same 5	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:18			0
15	BRS	L16	2227	beta-adrenergic adj receptor	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:19			0
16	BRS	L17	330	membrane adj transporter	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:20			0
17	BRS	L18	10687	(calcium or sodium or potassium) adj channel	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:20			0
18	BRS	L19	0	(16 or 17 or 18) same 6	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:21			0
19	BRS	L20	933	(16 or 17 or 18 or 7 or 8) same (binding adj site)	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:22			0

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21	BRS	L22	53312	(sulfhydryl adj reactive) or alkylating or acylating	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:24			0
22	BRS	L24	320315	methanethiosulfonyl or dithiopyridyl or disulfide or (halo adj ketone) or (diazo adj ketone) or anhydride or (active adj ester) or (pentafluorophenyl adj ester)	USPAT; US-PGPUB; EPO; JPO; DERWENT	2003/10/27 18:29			0
23	BRS	L25	263	(22 or 24) same anchoring	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:29			0
24	BRS	L26	1	1 same 25 same 5	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:29			0
25	BRS	L27	1	backx adj peter.in.	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:31			0
26	BRS	L28	5	dime adj david.in.	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:31			0
27	BRS	L29	1	kimmeldirk adj klaus.in.	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:31			0
28	BRS	L31	298	1 same target$3 same site-specific	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:32			0

	Type	L #	Hits	Search Text	DBs	Time Stamp	Comments	Error Definition	Errors
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30	BRS	L30	5	(27 or 28 or 29)	USPAT; US-PGPUB; EPO; JPO;	2003/10/27 18:33			0

2 parts common to all molecules

KAM 09/367,794

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L18             STR
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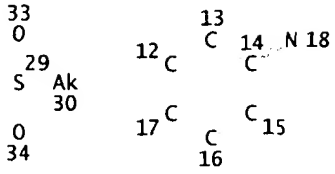


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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  13

STEREO ATTRIBUTES: NONE
L20           37 SEA FILE=REGISTRY SSS FUL L18
L21           20 SEA FILE=CAPLUS ABB=ON  PLU=ON  L20   20 cites

=> d ibib abs hitstr 1-20
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y


L21  ANSWER 1 OF 20  CAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2003:777393  CAPLUS
TITLE:                    Preparation of bi-valent inhibitors of viral de novo
                          RNA polymerases
INVENTOR(S):              Yao, Nanhua; An, Haoyun; Appleby, Todd; Nilar, Shahul;
                          Ding, Yili; Hong, Zhi
PATENT ASSIGNEE(S):       USA
SOURCE:                   U.S. Pat. Appl. Publ., 24 pp.
                          CODEN: USXXCO
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE           APPLICATION NO.  DATE
     ---------------   ----  --------       ---------------  --------
     US 2003187000      A1   20031002       US 2002-330369   20021227
PRIORITY APPLN. INFO.:                   US 2002-346680P  P  20020104
AB   A polymerase inhibitor has first moiety comprising a heterocyclic base
     coupled to a second moiety via an optional linker in which the first
     moiety binds to an initiation nucleotide binding site of a polymerase and
     forms at least two hydrogen bonds with an RNA template strand that is
     assocd. with the polymerase, and in which the second moiety comprised a
     compd. that binds to a site proximal to the nucleotide binding site of the
     polymerase and thereby increases the affinity of the polymerase inhibitor
     to the polymerase.  The polymerase target is an RNA-dependent RNA
     polymerase and more specifically is NS5B RNA-dependent RNA polymerase from
     hepatitis C virus.
IT   606972-32-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (prepn. of bi-valent inhibitors of viral de novo RNA polymerases)
RN   606972-32-1  CAPLUS
CN   INDEX NAME NOT YET ASSIGNED
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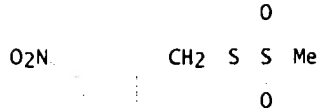
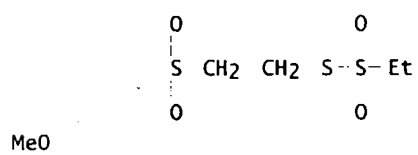


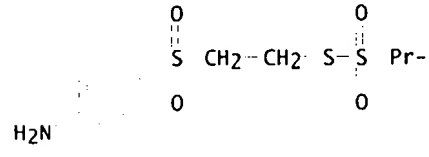
L21 ANSWER 2 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 2002:168085 CAPLUS
DOCUMENT NUMBER: 136:401346
TITLE: Synthesis of S-[arylsulfonylethyl] thiosulfonates and their alkaline hydrolysis
AUTHOR(S): Lubenets, V. I.; Baranovich, D. B.; Yarish, M. E.; Voloshinets, V. A.; Novikov, V. P.
CORPORATE SOURCE: Nats. Univ. "L'vivs'ka Politekhnika", Lvov, Ukraine
SOURCE: Ukrainskii Khimicheskii Zhurnal (Russian Edition) (2001), 67(11-12), 103-109
CODEN: UKZHAU; ISSN: 0041-6045
PUBLISHER: Institut Obshchei i Neorganicheskoi Khimii im. V. I. Vernadskogo NAN Ukrainy
DOCUMENT TYPE: Journal
LANGUAGE: Ukrainian

AB Alkylation of R3SO2SM (thiosulfonic acid alkali metal salts) by ArSO2(CH2)2OSO3Na afforded the corresponding thiosulfonates ArSO2(CH2)2SSO2R3; the alk. hydrolysis kinetics of the latter were reported.

IT **428862-17-3P**
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(synthesis of S-(arylsulfonylethyl) thiosulfonates and their alk. hydrolysis)
RN 428862-17-3 CAPLUS
CN Ethanesulfonothioic acid, S-[2-[(3-amino-4-methoxyphenyl)sulfonyl]ethyl] ester (9CI) (CA INDEX NAME)

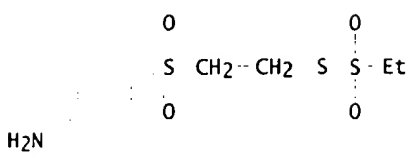


IT **428862-13-9P 428862-15-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of S-(arylsulfonylethyl) thiosulfonates and their alk. hydrolysis)
RN 428862-13-9 CAPLUS
CN 2-Propanesulfonothioic acid, S-[2-[(4-aminophenyl)sulfonyl]ethyl] ester (9CI) (CA INDEX NAME)



RN 428862-15-1 CAPLUS
CN Ethanesulfonothioic acid, S-[2-[(4-aminophenyl)sulfonyl]ethyl] ester (9CI)

(CA INDEX NAME)



L21 ANSWER 3 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:487228 CAPLUS
DOCUMENT NUMBER: 131:99258
TITLE: Chemically modified mutant enzymes, methods for producing and screening them, and their use as detergent and feed additives and for textile treatment
INVENTOR(S): Jones, J. Bryan; Plettner, Erika
PATENT ASSIGNEE(S): Genencor International, Inc., USA
SOURCE: PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9937323	A1	19990729	WO 1999-US1230	19990121
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2327254	AA	19990729	CA 1999-2327254	19990121
AU 9923308	A1	19990809	AU 1999-23308	19990121
EP 1064019	A1	20010103	EP 1999-903240	19990121
R: BE, DE, DK, ES, FR, GB, NL, SE, PT, FI				
US 6284512	B1	20010904	US 1999-234956	19990121
JP 2002500873	T2	20020115	JP 2000-528303	19990121
NZ 507344	A	20030829	NZ 1999-507344	19990121
US 2002012959	A1	20020131	US 2001-938801	20010824
US 2002015976	A1	20020207	US 2001-938940	20010824

PRIORITY APPLN. INFO.:
US 1998-72266P P 19980123
US 1998-872266 A 19980123
US 1999-234956 A3 19990121
WO 1999-US1230 W 19990121

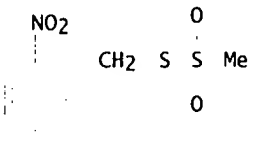
AB The present invention relates to method for screening chem. modified mutant enzymes for amidase and/or esterase activity. This method includes providing a chem. modified mutant enzyme with a substrate for an amidase and/or a substrate for an esterase and detg. whether the chem. modified mutant enzyme exhibits amidase and/or esterase activity. The present invention also relates to chem. modified mutant enzymes and a method for producing them where one or more amino acid residues from an enzyme are replaced by cysteine residues, and the cysteine residues are modified by replacing at least some of the thiol hydrogen in the cysteine residue with a thiol side chain to form the chem. modified mutant enzyme. The thiol side chain is selected from the group consisting of -SCH2(p-CH3-C6H4), -SCH2(p-OCH3-C6H4), -SCH2(p-CF3-C6H4), and -SCH2(2,4-diNO2-C6H3). The invention is demonstrated with Bacillus lentus subtilisin. After creating N62C, S166C, and L217C mutants, the newly created Cys residues were reacted with a series of phenylmethyl methanethiosulfonates. Some of the resulting derivs., esp. the mutants reacted with MeSO2SCH2(p-CO2H-C6H4),

had a favorably increased esterase:amidase ratio.

IT **215532-24-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(chem. modified mutant enzymes, methods for producing and screening them, and their use as detergent and feed additives and for textile treatment)

RN 215532-24-4 CAPLUS

CN Methanesulfonothioic acid, S-[(2,4-dinitrophenyl)methyl] ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

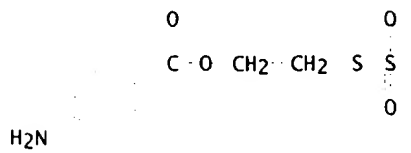
L21 ANSWER 4 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:437299 CAPLUS
DOCUMENT NUMBER: 131:208589
TITLE: Local anesthetic anchoring to cardiac sodium channels: implications into tissue-selective drug targeting
AUTHOR(S): Li, Ronald A.; Tsushima, Robert G.; Himmeldirk, Klaus; Dime, David S.; Backx, Peter H.
CORPORATE SOURCE: Departments of Physiology and Medicine, Centre for Cardiovascular Research, The Toronto Hospital, University of Toronto, Toronto, ON, Can.
SOURCE: Circulation Research (1999), 85(1), 88-98
CODEN: CIRUAL; ISSN: 0009-7330
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Local anesthetics inhibit Na+ channels in a variety of tissues, leading to potentially serious side effects when used clin. A series of novel local anesthetics was created by connecting benzocaine (BZ) to the sulfhydryl-reactive group methanethiosulfonate (MTS) via variable-length polyethylether linkers (L) (MTS-LX-BZ [X represents 0, 3, 6, or 9]). The application of MTS-LX-BZ agents modified native rat cardiac as well as heterologously expressed human heart (hH1) and rat skeletal muscle (rSkM1) Na+ channels in a manner resembling that of free BZ. Like BZ, the effects of MTS-LX-BZ on rSkM1 channels were completely reversible. In contrast, MTS-LX-BZ modification of heart and mutant rSkM1 channels, contg. a pore cysteine at the equiv. location as cardiac Na+ channels (i.e., Y401C), persisted after drug washout unless treated with DTT, which suggests anchoring to the pore via a disulfide bond. Anchored MTS-LX-BZ competitively reduced the affinity of cardiac Na+ channels for lidocaine but had minimal effects on mutant channels with disrupted local anesthetic modification properties. These results establish that anchored MTS-LX-BZ compds. interact with the local anesthetic binding site (LABS). Variation in the linker length altered the potency of channel modification by the anchored drugs, thus providing information on the spatial relationship between the anchoring site and the LABS. These observations demonstrate that local anesthetics can be anchored to the extracellular pore cysteine in cardiac Na+ channels and dynamically interact with the intracellular LABS. The results suggest that nonselective agents, such as local anesthetics, might be made more selective by linking these agents to target-specific anchors.

IT **212207-24-4 212261-85-3 243640-41-7**
243640-42-8
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(local anesthetic anchoring to cardiac sodium channels and implications

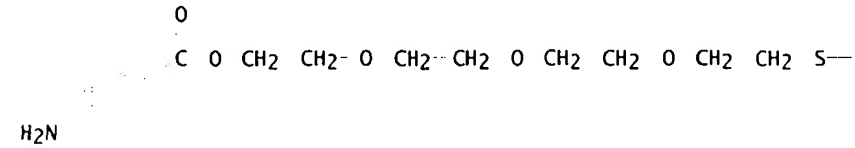
into tissue-selective drug targeting)

RN 212207-24-4 CAPLUS
CN Methanesulfonothioic acid, S-[2-[(4-aminobenzoyl)oxy]ethyl] ester (9CI) (CA INDEX NAME)



RN 212261-85-3 CAPLUS
CN Methanesulfonothioic acid, S-[13-(4-aminophenyl)-13-oxo-3,6,9,12-tetraoxatridec-1-yl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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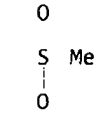
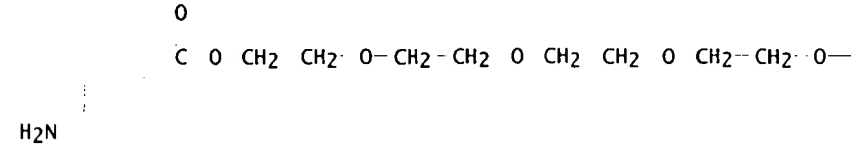


RN 243640-41-7 CAPLUS
CN Methanesulfonothioic acid, S-[22-(4-aminophenyl)-22-oxo-3,6,9,12,15,18,21-heptaoxadocos-1-yl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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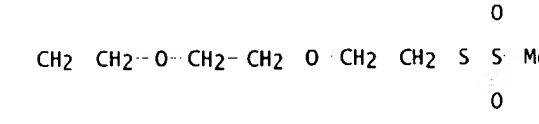
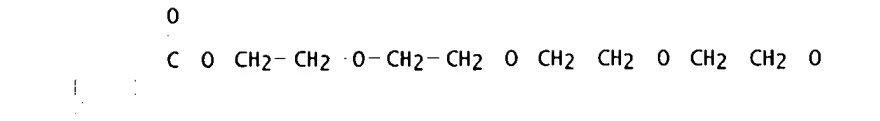


RN 243640-42-8 CAPLUS
CN Methanesulfonothioic acid, S-[31-(4-aminophenyl)-31-oxo-3,6,9,12,15,18,21,24,27,30-decaoxahentriacont-1-yl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



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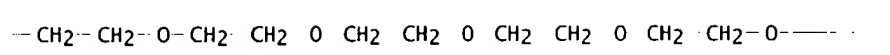
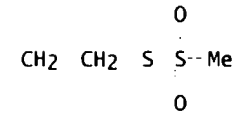


PAGE 1-C

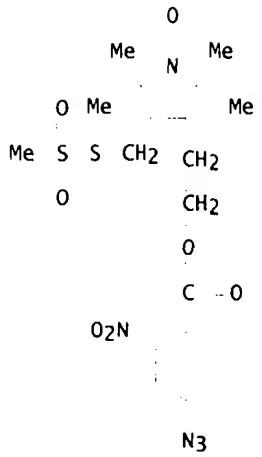


REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 5 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1999:361127 CAPLUS
DOCUMENT NUMBER: 131:181896
TITLE: Synthesis and Application of Novel Bifunctional Spin Labels
AUTHOR(S): Loesel, Ralf M.; Philipp, Reinhard; Kalai, Tamas; Hideg, Kalman; Trommer, Wolfgang E.
CORPORATE SOURCE: Fachbereich Chemie, Universitaet Kaiserslautern, Kaiserslautern, D-67653, Germany
SOURCE: Bioconjugate Chemistry (1999), 10(4), 578-582
CODEN: BCCHES; ISSN: 1043-1802
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

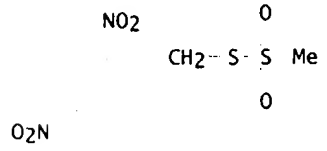
AB The synthesis of new bifunctional spin-labeled crosslinking reagents is described. Covalent attachment to papain was achieved via a thiol-specific thiosulfonate residue and, for the second anchor point, via a nonspecific photoreactive azido function. The thiosulfonate formed a reversible disulfide linkage, which could be cleaved again reductively by dithiothreitol. The spin label, a pyrroline-1-oxyl radical, was highly immobilized after attachment to papain by both functional groups and showed little if any relative motion with respect to the protein.

IT **240134-14-9P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(synthesis and application of novel bifunctional spin labels)
RN 240134-14-9 CAPLUS
CN 1H-Pyrrol-1-yloxy, 3-[2-[(4-azido-2-nitrobenzoyl)oxy]ethyl]-2,5-dihydro-2,2,5,5-tetramethyl-4-[[(methylsulfonyl)thio]methyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 6 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:630356 CAPLUS
DOCUMENT NUMBER: 129:341164
TITLE: A combinatorial approach to chemical modification of subtilisin Bacillus lentus
AUTHOR(S): Plettner, Erika; Khumtaveeporn, Kanjai; Shang, Xiao; Jones, J. Bryan
CORPORATE SOURCE: Department Chemistry, University Toronto, Toronto, ON, M5S 3H6, Can.
SOURCE: Bioorganic & Medicinal Chemistry Letters (1998), 8(17), 2291-2296
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The reaction between methanethiosulfonate reagents and cysteine mutants of subtilisin is quant. and can be used to prep. chem. modified mutant enzymes (CMMs) with novel properties. The virtually unrestricted structural variations possible for CMMs presents a preparative and screening challenge. To address this, a rapid combinatorial method for prepg. and screening the activities of CMMs has been developed.
IT **215532-24-4**
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); RCT (Reactant); BIOL (Biological study); RACT (Reactant or reagent); USES (Uses)
(combinatorial approach to chem. modification of subtilisin of Bacillus lentus)
RN 215532-24-4 CAPLUS
CN Methanesulfonothioic acid, S-[(2,4-dinitrophenyl)methyl] ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 7 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1998:604837 CAPLUS
DOCUMENT NUMBER: 129:221198
TITLE: Site-specific drug delivery
INVENTOR(S): Dime, David S.; Backx, Peter; Kimmeldirk, Klaus
PATENT ASSIGNEE(S): Can.
SOURCE: PCT Int. Appl., 72 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9836777	A1	19980827	WO 1998-CA133	19980219
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9862027	A1	19980909	AU 1998-62027	19980219
AU 735791	B2	20010712		
EP 966304	A1	19991229	EP 1998-903970	19980219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2001513081	T2	20010828	JP 1998-536114	19980219
NZ 337924	A	20020927	NZ 1998-337924	19980219

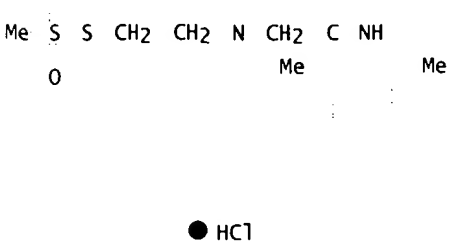
PRIORITY APPLN. INFO.: US 1997-42911P P 19970220
US 1997-66635P P 19971111
WO 1998-CA133 W 19980219

AB Compds. and methods which are useful for the site-specific delivery and localization of drugs are provided. The compds. can be represented by the formula: A-L-D wherein A is an anchoring moiety; L is a linking group; and D is a drug. E.g., 4-H2NC6H4CO2CH2CH2SSO2Me was prepd. from p-aminobenzoic acid and 2-hydroxyethyl methanethiosulfonate.

IT **212262-07-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(aminobenzoate methanethiosulfonates for site specific drug delivery)

RN 212262-07-2 CAPLUS

CN Methanesulfonothioic acid, S-[2-[[2-[(2,6-dimethylphenyl)amino]-2-oxoethyl]methylamino]ethyl] ester, monohydrochloride (9CI) (CA INDEX NAME)

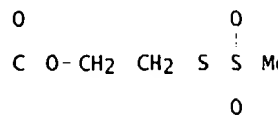


● HCl

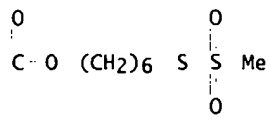
IT **212207-24-4P 212207-25-5P 212207-26-6P**
212207-27-7P 212207-28-8P 212261-85-3P
212261-87-5P 212261-88-6P 212261-89-7P
212261-90-0P 212261-91-1P
RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(aminobenzoate methanethiosulfonates for site specific drug delivery)

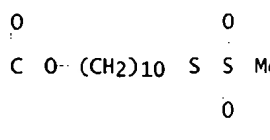
RN 212207-24-4 CAPLUS
CN Methanesulfonothioic acid, S-[2-[(4-aminobenzoyl)oxy]ethyl] ester (9CI) (CA INDEX NAME)



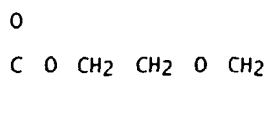
RN 212207-25-5 CAPLUS
CN Methanesulfonothioic acid, S-[6-[(4-aminobenzoyl)oxy]hexyl] ester (9CI) (CA INDEX NAME)



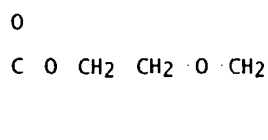
RN 212207-26-6 CAPLUS
CN Methanesulfonothioic acid, S-[10-[(4-aminobenzoyl)oxy]decyl] ester (9CI) (CA INDEX NAME)



RN 212207-27-7 CAPLUS
CN Methanesulfonothioic acid, S-[2-[2-[(4-aminobenzoyl)oxy]ethoxy]ethyl] ester (9CI) (CA INDEX NAME)



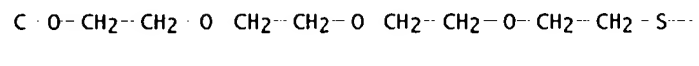
RN 212207-28-8 CAPLUS
CN Methanesulfonothioic acid, S-[2-[2-[2-[(4-aminobenzoyl)oxy]ethoxy]ethoxy]ethyl] ester (9CI) (CA INDEX NAME)



RN 212261-85-3 CAPLUS

CN Methanesulfonothioic acid, S-[13-(4-aminophenyl)-13-oxo-3,6,9,12-tetraoxatridec-1-yl] ester (9CI) (CA INDEX NAME)

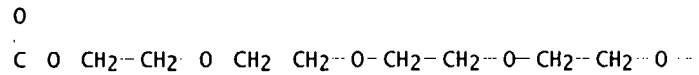
PAGE 1-A



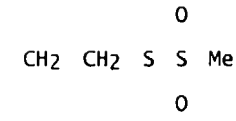
PAGE 1-B

RN 212261-87-5 CAPLUS
CN Methanesulfonothioic acid, S-[16-(4-aminophenyl)-16-oxo-3,6,9,12,15-pentaoxahexadec-1-yl] ester (9CI) (CA INDEX NAME)

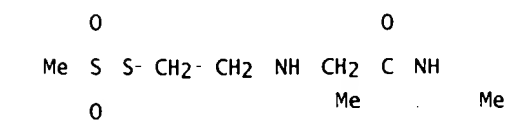
PAGE 1-A



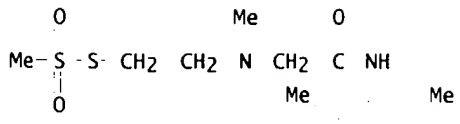
PAGE 1-B



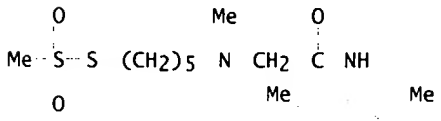
RN 212261-88-6 CAPLUS
CN Methanesulfonothioic acid, S-[2-[[2-[(2,6-dimethylphenyl)amino]-2-oxoethyl]amino]ethyl] ester (9CI) (CA INDEX NAME)



RN 212261-89-7 CAPLUS
CN Methanesulfonothioic acid, S-[2-[[2-[(2,6-dimethylphenyl)amino]-2-oxoethyl]methylamino]ethyl] ester (9CI) (CA INDEX NAME)

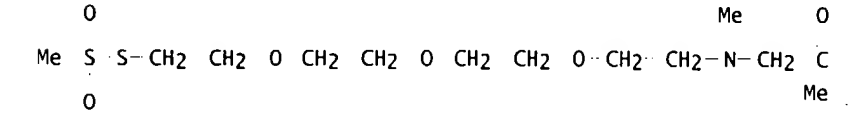


RN 212261-90-0 CAPLUS
CN Methanesulfonothioic acid, S-[5-[[2-[(2,6-dimethylphenyl)amino]-2-oxoethyl]methylamino]pentyl] ester (9CI) (CA INDEX NAME)

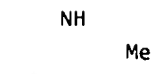


RN 212261-91-1 CAPLUS
CN Methanesulfonothioic acid, S-[14-[(2,6-dimethylphenyl)amino]-12-methyl-17-oxo-3,6,9-trioxa-12-azatetradec-1-yl] ester (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B



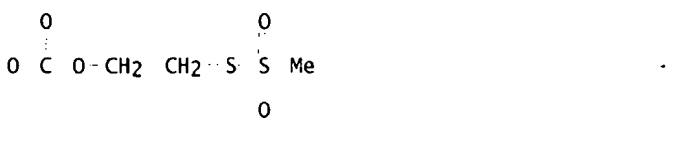
REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L21 ANSWER 8 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1997:67716 CAPLUS
DOCUMENT NUMBER: 126:183455
TITLE: Development of a Novel Thiol Reagent for Probing Ion Channel Structure: Studies in a Model System
AUTHOR(S): Foong, Louise Y.; You, Shaochun; Jaikaran, Dominic C. J.; Zhang, Zhihua; Zunic, Valentin; Woolley, G. Andrew
CORPORATE SOURCE: Lash Miller Chemical Laboratories Department of Chemistry, University of Toronto, Toronto, ON, M5S 3H6, Can.
SOURCE: Biochemistry (1997), 36(6), 1343-1348
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We have synthesized a novel thiol reagent, 2-[(methylsulfonyl)thio]ethyl

[N-(N,N-dimethylamino)ethyl]carbamate (MTSAC), that contains a carbamate functional group as well as a (pos. charged) terminal amino group. The carbamate C-N bond isomerizes on a millisecond time scale and significantly alters the three-dimensional shape of the reagent. The behavior of this reagent was contrasted with that of the commonly used thiol reagent, [(methylsulfonyl)thio]ethylamine MTSEA [Akabas, M. H., & Karlin, A. (1995) Biochem. 34, 12496-12500], with respect to its effect on single-channel currents passing through modified gramicidin channels. While both reagents decreased single-channel currents, the MTSAC-treated channels also showed a pattern of steps in the current recordings on the time scale of the carbamate bond isomerization. Moreover, the pattern and size of these steps were sensitive to the location of the thiol-reactive site in relation to the channel entrance. Thus, MTSAC may prove useful as a reagent for establishing the proximity to the pore in studies of ion channel proteins of unknown structure.

IT **187592-55-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(development of a novel thiol reagent for probing ion channel structure)

RN 187592-55-8 CAPLUS
CN Methanesulfonothioic acid, S-[2-[[(4-nitrophenoxy)carbonyl]oxy]ethyl] ester (9CI) (CA INDEX NAME)

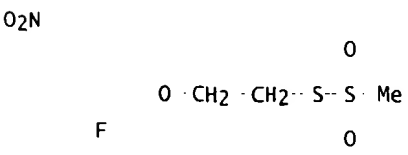


L21 ANSWER 9 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1990:21268 CAPLUS
DOCUMENT NUMBER: 112:21268
TITLE: Nucleophilic group selective photolabeling reagents
AUTHOR(S): Hatanaka, Yasumaru; Yoshida, Eiichi; Taki, Motohiko; Nakayama, Hitoshi; Kanaoka, Yuichi
CORPORATE SOURCE: Fac. Pharm. Sci., Hokkaido Univ., Japan
SOURCE: *Photomedicine and Photobiology* (1988), 10, 215-16
CODEN: PHPHEA; ISSN: 0912-232X
DOCUMENT TYPE: Journal
LANGUAGE: English

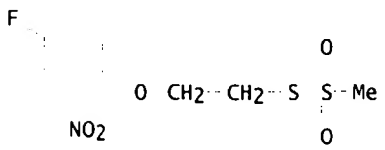
AB The prepn. and potential use of fluoronitroanisoles as photolabeling reagents are reported. In model protein systems, RR1C6H3OMe (R = 2-F, R1 = 4-NO2; R = 2-NO2, R1 = 4-F) underwent photochem. substitution with Ac-Lys-NH2 and 2,4-R3R4C6H3OCH2CH2SSO2Me (R3 = F, R4 = NO3; R3 = NO3, R4 = F) underwent photochem. reaction with glyceraldehyde-3-phosphate dehydrogenase.

IT **124395-12-6P 124395-13-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and photochem. reaction of, with glyceraldehyde-3-phosphate dehydrogenase, labeling by)

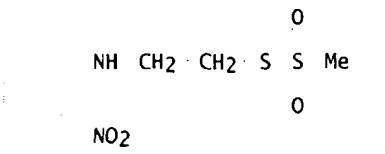
RN 124395-12-6 CAPLUS
CN Methanesulfonothioic acid, S-[2-(2-fluoro-4-nitrophenoxy)ethyl] ester (9CI) (CA INDEX NAME)



RN 124395-13-7 CAPLUS
CN Methanesulfonothioic acid, S-[2-(4-fluoro-2-nitrophenoxy)ethyl] ester (9CI) (CA INDEX NAME)



L21 ANSWER 10 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1986:164608 CAPLUS
DOCUMENT NUMBER: 104:164608
TITLE: A fluorogenic, mixed-disulfide reagent for thiol assay
AUTHOR(S): Willis, Kevin J.; Teale, Francis W. J.
CORPORATE SOURCE: Dep. Biochem., Univ. Birmingham, Birmingham, B15 2TT, UK
SOURCE: Analytical Biochemistry (1986), 153(2), 336-47
CODEN: ANBCA2; ISSN: 0003-2697
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The design and synthesis of the mixed disulfide (o-nitroanilide-N-ethyldithio)2-[pyridyl-5-thioureido-N'-(5-fluorescein)] are described and the chem. and spectroscopic properties of this thiol-specific fluorogenic reagent are presented. The high reactivity and sensitivity of this reagent in thiol assay are demonstrated with low-mol.-wt. thiols and with human carbonmonoxyHb and its subunits and sperm-whale myoglobin. Comparison with conventional absorption methods shows that at least 100 times less material is needed; moreover, high background absorbance or turbidity do not interfere with the assay.
IT **101559-39-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with fluoronitrobenzene)
RN 101559-39-1 CAPLUS
CN Methanesulfonothioic acid, S-[2-[(2-nitrophenyl)amino]ethyl] ester (9CI) (CA INDEX NAME)



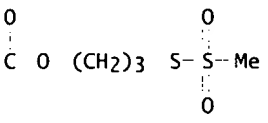
L21 ANSWER 11 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1981:24512 CAPLUS
DOCUMENT NUMBER: 94:24512
TITLE: Gas chromatographic and gas chromatographic-mass spectrometric characterization of methanethiosulfonates carrying further functional groups
AUTHOR(S): Corina, David L.; Bloxham, David P.; Cooper, Gary K.
CORPORATE SOURCE: Sch. Biochem. Physiol. Sci., Univ. Southampton, Southampton, SO9 3TU, UK
SOURCE: Journal of Chromatography (1980), 198(3), 287-92
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A group of methanethiosulfonates was characterized by gas chromatog. (GC) and GC-mass spectrometry (MS). These compds. contain addnl. functional

groups and have the general structure MeSO2S(CH2)nR and MeSO2SCH2CO(CH2)nR (where R is an O-contg. group). Although in a few cases some decompn. on GC to the resp. sulfones was obsd., all samples gave characteristic mass spectra and all but one could be characterized by combined GC-MS. Certain aspects of the GC and MS behavior are briefly discussed.

IT **76091-05-9**
RL: PRP (Properties); ANST (Analytical study)
(gas chromatog. and mass spectroscopy of)

RN 76091-05-9 CAPLUS

CN Benzoic acid, 4-azido-, 3-[(methylsulfonyl)thio]propyl ester (9CI) (CA INDEX NAME)



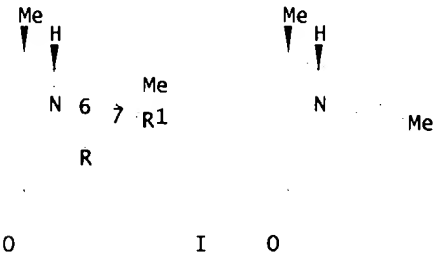
L21 ANSWER 12 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1976:577750 CAPLUS
DOCUMENT NUMBER: 85:177750
TITLE: Pharmaceutical compositions containing nupharidine derivatives
INVENTOR(S): LaLonde, Robert T.; Tsai, Amy I. M.; Wang, Chun Juan; Wong, Chunfook
PATENT ASSIGNEE(S): Research Corp., USA
SOURCE: Ger. Offen., 27 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2603140	A1	19760805	DE 1976-2603140	19760128
US 4011327	A	19770308	US 1975-546191	19750131
SE 7601022	A	19760801	SE 1976-1022	19760130
JP 51101999	A2	19760908	JP 1976-9936	19760131
FR 2299030	A1	19760827	FR 1976-2718	19760202

PRIORITY APPLN. INFO.: US 1975-546191 19750131

GI



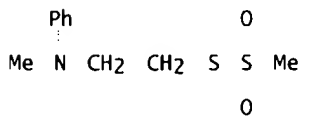
AB Thiodeoxynupharidinols I (R = HO, AcO; R1 = alkylthio, cyclohexylthio, alkenylthio, alkoxycarbonylmethylthio) and the resp. 6.beta.,7.alpha.-I (25 compds.), possessing fungicidal activity, were prepd. by condensing dehydrodeoxynupharidine (II) with R2SO2SR1 (R2 = Me, Ph, 4-MeC6H4, cyclohexyl). Thus, a C6H6 soln. of II was treated with 4-MeC6H4SO2SMe at 25.degree. under N in the presence of alumina to give I (R = HO, R1 = MeS)

(III) and 6.beta.,7.alpha.-III.

IT **60929-88-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dehydrodeoxynupharidine)

RN 60929-88-6 CAPLUS

CN Methanesulfonothioic acid, S-[2-(methylphenylamino)ethyl] ester (9CI) (CA INDEX NAME)



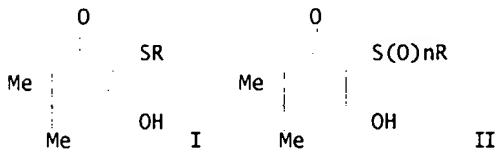
L21 ANSWER 13 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1976:446084 CAPLUS
DOCUMENT NUMBER: 85:46084
TITLE: 2-(Sulfur-substituted)-3-hydroxy-5,5-dimethyl-2-cyclohexen-1-ones
INVENTOR(S): Dunbar, Joseph E.; Bohnert, Thomas J.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: U.S., 7 pp. Division of U.S. 3,852,359.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3943176	A	19760309	US 1974-466596	19740503
US 3852359	A	19741203	US 1972-319361	19721229

PRIORITY APPLN. INFO.: US 1972-319361 19720229

GI

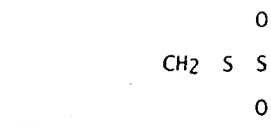


AB 5,5-Dimethyl-3-hydroxy-2-cyclohexenone reacted with R1SO2SR (R1 = p-tolyl, Me; R = C3-5 alkyl, allyl, substituted allyl, cyclohexylmethyl, CH2CH2SMe, PhCH2, substituted benzyl) to give twelve resp. 1-oxo-2-cyclohexen-2-yl sulfides I which exhibited plant growth regulator activity. Six I were oxidized to II (n = 1,2), which also showed the above activity.

IT **53291-36-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction of, with 3-hydroxy-2-cyclohexenone deriv.)

RN 53291-36-4 CAPLUS

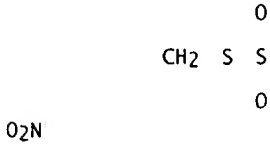
CN Methanesulfonothioic acid, S-[(4-nitrophenyl)methyl] ester (9CI) (CA INDEX NAME)



L21 ANSWER 14 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1976:16862 CAPLUS
DOCUMENT NUMBER: 84:16862
TITLE: 2-(Sulfur-substituted)-3-hydroxy-5,5-dimethyl-2-cyclohexen-1-ones
INVENTOR(S): Dunbar, Joseph E.; Bohnert, Thomas J.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: U.S., 8 pp. Division of U.S. 3,852,359.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3914316	A	19751021	US 1974-438929	19740201
US 3852359	A	19741203	US 1972-319361	19721229

PRIORITY APPLN. INFO.: US 1972-319361 19721229
GI For diagram(s), see printed CA Issue.
AB 5,5-Dimethyl-3-hydroxy-2-cyclohexen-1-one reacted with R1SO2SR (R = alkyl, alkenyl, cyclohexylmethyl, substituted benzyl, PhCH2; R1 = Me, p-tolyl) and NaOH to give fourteen resp. sulfides (I, n = 0), which exhibited plant growth regulation activity. seven sulfides were oxidized to the resp. sulfoxide (I, n = 1), which were also effective as plant regulators.
IT **53291-36-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with 3-hydroxy-2-cyclohexenone deriv.)
RN 53291-36-4 CAPLUS
CN Methanesulfonothioic acid, S-[(4-nitrophenyl)methyl] ester (9CI) (CA INDEX NAME)



L21 ANSWER 15 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1975:563712 CAPLUS
DOCUMENT NUMBER: 83:163712
TITLE: 2-(Sulfur-substituted)-3-hydroxy-5,5-dimethyl1-2-cyclohexen-1-ones
INVENTOR(S): Dunbar, Joseph E.; Bohnert, Thomas J.
PATENT ASSIGNEE(S): Dow Chemical Co.
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

US 3852359	A	19741203	US 1972-319361	19721229
US 3914316	A	19751021	US 1974-438929	19740201
US 3943176	A	19760309	US 1974-466596	19740503

PRIORITY APPLN. INFO.: US 1972-319361 19721229

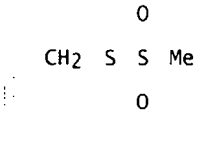
GI For diagram(s), see printed CA Issue.

AB The cyclohexenones I (R = CHMe2, allyl, CH2CCl:CH2, CH2CH:CMe2, CH2CH2SMe, cyclohexylmethyl, Me2CHCH2, Me2CHCH2CH2, p-ClC6H4CH2, p-FC6H4CH2, p-O2NC6H4CH2, p-MeC6H4CH2, PhCH2, useful as plant growth regulators, were prepd. by reaction of 3-hydroxy-5,5-dimethyl-2-cyclohexen-1-one with R1SO2SR (R1 = p-tolyl, Me) in the presence of base,. The sulfoxides II (R = cyclohexylmethyl, Me2CHCH2, Me2CHCH2CH2, p-ClC6H4CH2, p-FC6H4CH2, p-MeC6H4CH2, benzyl) and the sulfones III (R = p-ClC6H4CH2, benzyl) were prepd. by oxidn. of the corresponding I.

IT **53291-36-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydroxydimethylcyclohexenone)

RN 53291-36-4 CAPLUS

CN *Methanesulfonothioic acid*, S-[(4-*nitrophenyl*)*methyl*] ester (9CI) (CA INDEX NAME)



L21 ANSWER 16 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1974:449568 CAPLUS

DOCUMENT NUMBER: 81:49568

TITLE: Sulfur-containing 4-hydroxycoumarins and their salts

INVENTOR(S): Dunbar, Joseph E.

PATENT ASSIGNEE(S): Dow Chemical Co.

SOURCE: U.S., 6 pp.
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: *English*

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3810922	A	19740514	US 1972-316419	19721218

PRIORITY APPLN. INFO.: US 1972-316419 19721218

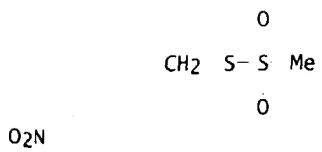
GI For diagram(s), see printed CA Issue.

AB Twenty-five coumarins I (R = Me, Me2CHCH2-CH2, Me(CH2)11, CH2:CHCH2, Me2CH, PhCH2, etc., n = 0, 1, 2) were prepd. Thus, 4-hydroxycoumarin was treated with p-MeC6H4SO2SCHMe2 and NaOH to give I (R = Me2CH, n = 0), which was oxidized with 30% H2O2 to give I (n = 1). In pre-emergence application at 10 lb/acre I (R = Me2CHCH2CH2, n = 0) (II) reduced yellow foxtail by 95%. The min. growth in-hibitory concn. of II against Mycobacterium phlei was 100 ppm.

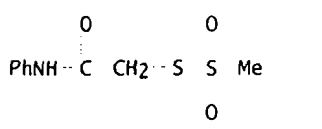
IT **53291-36-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with 4-hydroxycoumarin)

RN 53291-36-4 CAPLUS

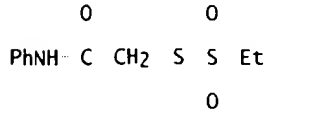
CN Methanesulfonothioic acid, S-[(4-nitrophenyl)methyl] ester (9CI) (CA INDEX NAME)



L21 ANSWER 17 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1968:21644 CAPLUS
DOCUMENT NUMBER: 68:21644
TITLE: Thiosulfonic acids. XVII. Derivatives of carboxymethyl esters of thiosulfonic acids
AUTHOR(S): Grivnak, L. M.; Boldyrev, B. G.
CORPORATE SOURCE: L'vovsk. Politekh. Inst., Lvov, USSR
SOURCE: Probl. Poluch. Poluprod. Prom. Org. Sin., Akad. Nauk SSSR, Otd. Obshch. Tekh. Khim. 1967 (1967), 77-80
CODEN: 16XSAS
DOCUMENT TYPE: Conference
LANGUAGE: Russian
AB RSO2SCH2COR' (I) were prepd. by treatment of RSO2SK with BrCH2COR' in aq. Me2CO at room temp. Prepd. were the following I (R, R', yield, and m.p. given): Me, EtO, 56.3%, -; Me, PhCH2NH, 69.0%, 76-7.degree.; Me, PhNH, 59.0%, 96-8.degree.; Et, MeO, 59.5%, -, Et, EtO, 77.0%, -; Et, PhO, 52.4%, -; Et, NH2, 68.9%, 61-3.degree.; Et, Et2N, 45.5%, -; Et, PhCH2NH, 72.0%, 73-4.degree.; Et, PhNH, 65.0%, 95-7.degree.; Ph, MeO, 76.0%, -; Ph, EtO, 73.5%, -; Ph, NH2, 64.0%, 108-9.degree.; Ph, PhCH2NH, 68.0%, 111-12.degree.; Ph, PhNH, 49.6%, 99-100.degree.; 4-ClC6H4, EtO, 74.3%, -; 4-ClC6H4, NH2, 72.4, 116-18.degree.; 4-ClC6H4, PhCH2NH, 69.0%, 89-90.degree.; 4-ClC6H4, PhNH, 80.0%, 112-13.degree.; 4-AcNHC6H4, MeO, 40.0%, 105-6.degree.; 4-AcNHC6H4, EtO, 57.0%, 71-2.degree.; 4-AcNHC6H4, PhO, 70.0%, 76-7.degree.; 4-AcNHC6H4, NH2, 71.7%, 150-1.degree.; 4-AcNHC6H4, PhNH, 71.5%, 165-6.degree.; 4-H2NC6H4, MeO, 71.8%, 93-4.degree.; 4-H2NC6H4, EtO, 73.0%, 92-3.degree.; 4-H2NC6H4, Et2N, 52.5%, 145-6.degree.; 4-AcNHC6H4, PhNH, 95.7%, 137-8.degree..
IT **16599-46-5P 16599-53-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 16599-46-5 CAPLUS
CN Methanesulfonic acid, thio-, S-ester with 2-mercaptoacetanilide (8CI) (CA INDEX NAME)



RN 16599-53-4 CAPLUS
CN Ethanesulfonic acid, thio-, S-ester with 2-mercaptoacetanilide (8CI) (CA INDEX NAME)



L21 ANSWER 18 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1967:516715 CAPLUS

DOCUMENT NUMBER: 67:116715
TITLE: .beta.,.beta.'-Bis(substituted sulfonylthio) compounds
INVENTOR(S): Dunbar, Joseph E.
PATENT ASSIGNEE(S): Dow Chemical Co.
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

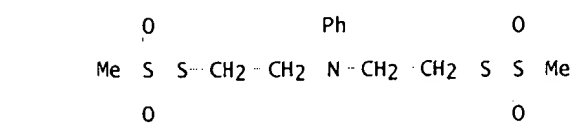
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3338945		19670829	US	19631025

AB [RSO2S(CH2)2]2 X, where R is lower alkyl, Ph, benzyl, halophenyl, methoxyphenyl, lower alkylphenyl, or alkylhalophenyl, X is O, S, SO, SO2, NR1, or NR1R2 in which R1 is H, C1-12 alkyl, Ph, halophenyl, loweralkylphenyl, alkoxyphenyl, cyclohexyl, bicyclo[2.2.1]-5-hepten-2-ylmethyl, or cyclooctyl, and R2 is HCl, HBr, or HI, were prepd. for use as pesticides. .beta.,.beta.'-Bis(methylsulfonylthio)diethyl ether, m. 71.5-2.5.degree. (MeOH), was obtained by heating 69.6 g. .beta.,.beta.'-dibromodiethyl ether (I) and 90.2 g. K methanethiosulfonate in 120 ml. dimethylformamide at 95.degree. for 1 hr., cooling, and dilg. with 1800 ml. ice-H2O. Similarly .beta.,.beta.'-bis(p-tolylsulfonylthio)diethyl ether, m. 60-1.degree. (MeOH), was obtained from 17.4 g. I and 34.0 g. K p-toluenethiosulfonate (II) in 35 ml. dimethylformamide; .beta.,.beta.'-bis(p-bromophenylsulfonylthio)diethyl ether, m. 71-4.degree., from 11.6 g. I and 29.1 g. K p-bromobenzenethiosulfonate (III) in 300 ml. EtOH refluxed for 16 hrs. Substitution of .beta.,.beta.'-dibromodiethyl sulfide for I gave bis[2-(p-bromophenylsulfonylthio)ethyl]sulfide, m. 89-91.degree., and bis[2-(p-methoxyphenylsulfonylthio)ethyl] sulfide, n25D 1.6251. N,N-bis[.beta.-(ethylsulfonylthio)ethyl]-tert-butylamine, m. 49-51.degree., was prepd. by refluxing 14.9 g. N,N-bis(2-chloroethyl)-tert-butylamine) (IV), 24.8 g. K ethanethiosulfonate, and 250 ml. EtOH; N,N-bis[.beta.-(4-bromophenylsulfonylthio)ethyl]-tert-butylamine, m. 119.5-21.5.degree. from III and IV. A mixt. of N,N-bis(2-chloroethyl)-tert-butylamine-HCl and II yielded N,N-bis[.beta.-(p-tolylsulfonylthio)ethyl]-tert-butylamine-HCl, m. 151.5-53.degree.. Bis[2-(p-tolylsulfonylthio)ethyl] sulfoxide, m. 82-5.degree., was obtained from 8.98 g. .beta.,.beta.'-dibromodiethyl sulfoxide and 15.2 g. II in 75 ml. EtOH; bis[2-(3,4-dichlorophenylsulfonylthio)ethyl] sulfone, m. 139-40.degree., from K 3,4-dichlorobenzenethiosulfonate and bis(2-bromoethyl) sulfone; N,N-bis[.beta.-(p-tolylsulfonylthio)ethyl]cyclohexylamine-HCl, m. 92-9.degree., from N,N-bis(2-chloroethyl)cyclohexylamine-HCl and II; N,N-bis[.beta.-(4-bromophenylsulfonylthio)ethyl]cyclooctylamine, m. 113-15.degree., from N,N-bis(2-chloroethyl)cyclooctylamine and III. Also prepd. were (m.p. given): .beta.,.beta.'-bis(phenylsulfonylthio)diethyl ether, 73.5-5.0.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]-n-dodecylamine, 48-50.degree.; N,N-bis[.beta.-(benzylsulfonylthio)ethyl]-tert-butylamine, 103-5.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]-tert-butylamine hydrochloride, 174-5.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]amine, 67.5-8.5.degree.; N,N-bis[.beta.-(phenylsulfonylthio)ethyl]-tert-butylamine, 90-2.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]-tert-butylamine, 72.5-5.5.degree.; bis[2-(2,5-dimethylphenylsulfonylthio)ethyl] sulfide, -(n25D1.6147); N,N-bis[.beta.-(p-tolylsulfonylthio)ethyl]-tert-butylamine, 87.5-89.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]methylamine, 144-6.degree.; .beta.,.beta.'-bis(2,5-dimethylphenylsulfonylthio)diethyl ether, 77-9.degree.; bis[2-(p-bromophenylsulfonylthio)ethyl] sulfide, 89-91.degree.; bis[2-(methylsulfonylthio)ethyl] sulfide, 77-8.degree.; bis[2-(phenylsulfonylthio)ethyl] sulfide, 75-7.degree.; bis[2-(p-tolylsulfonylthio)ethyl] sulfide, 55.5-6.5.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]aniline, 120-3.degree.; bis[2-phenylsulfonylthio)ethyl] sulfoxide, 78-80.degree.; bis[2-(p-bromophenylsulfonylthio)ethyl] sulfoxide, 124-6.degree.;

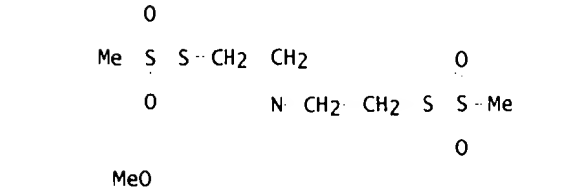
bis[2-(p-fluorophenylsulfonylthio)ethyl] sulfoxide, 98-100.5.degree.; bis[2-(3,4-dichlorophenylsulfonylthio)ethyl] sulfoxide, 127.5-29.degree.; bis[2-(methylsulfonylthio)ethyl] sulfone, 123.5-4.5.degree.; bis[2-(ethylsulfonylthio)ethyl] sulfone, 101-102.degree.; bis[2-(butylsulfonylthio)ethyl] sulfone, 99-9.5.degree.; bis[2-(phenylsulfonylthio)ethyl] sulfone, 144-6.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]cyclohexylamine-HCl, 127.5-29.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]cyclohexylamine, 80-2.degree.; N,N-bis[.beta.-(p-tolylsulfonylthio)ethyl]cyclohexylamine, 115.5-17.5.degree.; N,N-bis-[.beta.-(phenylsulfonylthio)ethylcyclohexylamine, 72-4.degree.; N,N-bis[.beta.-(3,4-dichlorophenylsulfonylthio)ethyl]cyclohexylamine, 153-4.5.degree.; N,N-bis[.beta.-(n-butylsulfonylthio)ethyl]cyclohexylamine-HCl, 152-4.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]cyclooctylamine, 72-4.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]cyclooctylamine-HCl, 156.5-58.degree.; N,N-bis[.beta.-(ethylsulfonylthio)ethyl]cyclooctylamine, 48-9.degree.; N,N-bis[.beta.-(phenylsulfonylthio)ethyl]cyclooctylamine, 69-71.degree.; N,N-bis[.beta.-(p-tolylsulfonylthio)ethyl]cyclooctylamine, 105-6.5.degree.; N,N-bis[.beta. - (4 - bromophenylsulfonylthio)ethyl]cyclooctylamine - HCl, 165.5.degree. (decompn.); N,N-bis[.beta.-(2,5-dimethylphenylsulfonylthio)ethyl]cyclooctylamine-HCl, 133-5.degree. (decompn.); N,N-bis[.beta.-(methylsulfonylthio)ethyl]-n-dodecylamine, 50.5-53.degree.; N,N-bis[.beta.-(p-tolylsulfonylthio)ethyl]-n-dodecylamine, n25D 1.5305; N,N-bis[.beta.-(methylsulfonylthio)ethyl]bicyclo[2.2.1] - 5 - hepten - 2 - yl-methylamine-HCl, 73.degree. (decompn.); N,N-bis[.beta.-methylsulfonylthio)ethyl]-2,6-dimethylaniline, 77.5-9.5.degree.; N,N-bis[.beta.-(methylsulfonylthio)ethyl]-p-methoxyaniline, 98.5-99.degree.. As pesticides, .beta.,.beta.'-bis(phenylsulfonylthio)diethyl ether, .beta.,.beta.'-bis(p-tolylsulfonylthio)diethyl ether, bis[2-(methylsulfonylthio)ethyl] sulfide, and N,N-bis[.beta.-ethylsulfonylthio)ethyl]-tert-butylamine each gave complete control of Aerobacter aerogenes, Pseudomonas aeruginosa, Salmonella typhosa, and Staphylococcus aureus at 1000 ppm. .beta.,.beta.'-bis(methylsulfonylthio)diethyl ether at 500 ppm. controlled late blight, while N,N-bis[.beta.-(phenylsulfonylthio)ethyl]cyclooctylamine at 500 ppm. killed bacterium fire blight, Bacillus cereus, and S. aureus.

IT **15994-51-1P 16186-80-4P 16216-84-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

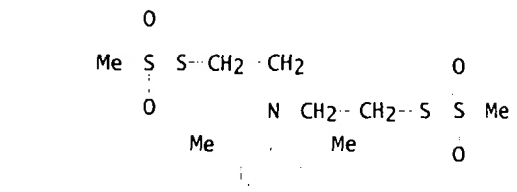
RN 15994-51-1 CAPLUS
CN Methanesulfonic acid, thio-, S,S'-[(phenylimino)diethylene] ester (8CI) (CA INDEX NAME)



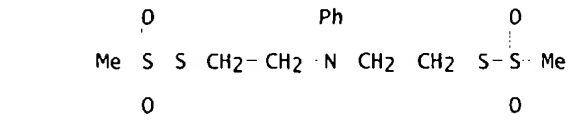
RN 16186-80-4 CAPLUS
CN Methanesulfonic acid, thio-, S,S'-[[(p-methoxyphenyl)imino]diethylene] ester (8CI) (CA INDEX NAME)



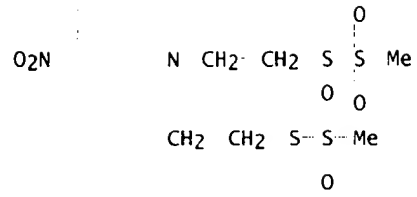
RN 16216-84-5 CAPLUS
CN Methanesulfonic acid, thio-, S,S'-[(2,6-xylylimino)diethylene] ester (8CI) (CA INDEX NAME)



L21 ANSWER 19 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1967:490748 CAPLUS
DOCUMENT NUMBER: 67:90748
TITLE: Reaction of the thiosulfonate group with the aromatic nucleus: a new ring closure
AUTHOR(S): Dunbar, Joseph E.; Tarnowski, Betty H.
CORPORATE SOURCE: Edgar C. Britton Res. Lab., Dow Chem. Co., Midland, MI, USA
SOURCE: Journal of Heterocyclic Chemistry (1967), 4(3), 339-43
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The double ring closure of N,N-bis[(2-alkyl- or arylsulfonylthio)ethyl]anilines to form 2,3,5,6-tetrahydro[1,4]thiazino[4,3,2-de][1,4]benzothiazines (I), a new ring system, is reported. The effects of various benzene ring substituents upon the ring closure are described.
IT **15994-51-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)
RN 15994-51-1 CAPLUS
CN Methanesulfonic acid, thio-, S,S'-[(phenylimino)diethylene] ester (8CI) (CA INDEX NAME)



IT **15994-57-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 15994-57-7 CAPLUS
CN Methanesulfonic acid, thio-, S,S'-[[(m-nitrophenyl)imino]diethylene] ester (8CI) (CA INDEX NAME)



L21 ANSWER 20 OF 20 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1966:35631 CAPLUS
DOCUMENT NUMBER: 64:35631
ORIGINAL REFERENCE NO.: 64:6566b-f
TITLE: Carbamate thiosulfonates
INVENTOR(S): Dunbar, Joseph E.
PATENT ASSIGNEE(S): Dow Chemical Co.
SOURCE: 3 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3226427		19651228	US	19631028

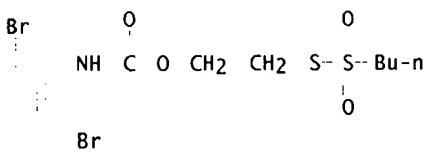
AB The reaction is described of o-halo-alkyl carbamates such as 2-bromoethyl (I), ethylene, or 3-bromopropyl N-phenylcarbamate, 2-bromoethyl N-methyl-, 3-bromopropyl N-(3,5-dibromophenyl)-, 2-bromoethyl N-(pentachlorophenyl)-, 2-iodoethyl N-hexyl-, 2-bromoethyl N-(2,4,6-tribromophenyl)-, 3-bromopropyl N-(2,5 dichlorophenyl), 2-iodoethyl N-(pentamethylphenyl)-, 3-bromopropyl N-(3,5-dimethyl-4-bromophenyl)-, and 2-bromomethyl N-(p-pentylphenyl)carbamate with an alkali metal salt of a thiosulfonic acid such as K methane- (II), K p-toluene-, K p-bromobenzene-, K (3-methyl-5-chlorobenzene)-, K pentachlorobenzene-, K hexyl-, K butane-, K benzene-Na 3,5-dibromo-6-methylbenzene-, K 3-iodobenzene-K 2,6-dibromobenzene- and Na 2-chloro-5-(2-methylpentyl)benzenethiosulfonate in the presence of a solvent or diluent such as HCONMe2 (DMF) at 55-100.degree. to obtain the title compds. For example, I 7.33 and II 4.51 g. were dispersed in 20 ml. DMF and the mixt. was heated with stirring 40 min. at 95.degree., then cooled to room temp. and filtered. The filtrate was dild. with H2O and the org. layer which sepd. allowed to stand in contact with the aq. layer for several hrs. at room temp. during which time it solidified to give ethylenemethanethiosulfonate N-phenylcarbamate, PhNHCO2CH2CH2SSO2Me (III), m. 58-9.degree. (EtOH). Similarly prepd. were ethylene-p-toluenethiosulfonate, N-phenylcarbamate, PhNHCO2CH2CH2SSO2C6H4Me (IV), m. 85-7.degree. (EtOH); ethylene-p-bromobenzenethiosulfonate N-phenylcarbamate, m. 97.5-100.degree.; ethylenemethanethiosulfonate N-methylcarbamate (V), m. 70-2.degree. (iso-PrOH); trimethylene-3-methyl-5-chlorobenzenethiosulfonate N-(3,5-dibromophenyl)carbamate; ethylenepentachlorobenzenethiosulfonate N-(pentachlorophenyl)carbamate; trimethylenemethanesulfonate N-phenylcarbamate (VI), m. 58-60.degree.; ethylenehexanethiosulfonate N-hexylcarbamate; ethylenebutanethiosulfonate N-(2,4,6-tribromophenyl)carbamate, m. 52-4.degree.; ethylenebenzenethiosulfonate N-phenylcarbamate, m. 60.5-2.5.degree.; trimethylene(3,5-dibromo-6-methylbenzene)thiosulfonate N-(2,5-dichlorophenyl)carbamate; ethylene(3-iodobenzene)thiosulfonate N-(pentamethylphenyl)carbamate; trimethylene(2,6-dibromobenzene)thiosulfonate N-(3,5-dimethyl-4-bromophenyl)carbamate; ethylene [2-chloro-5-(2-methylpentyl)phenyl] thiosulfonate N-(p-pentylphenyl)carbamate; and ethylenebutanethiosulfonate N-phenylcarbamate (VII). Compns. contg. 2 ppm. by vol. of V produced 100% kill of lake emerald shiner. Excellent kill and control of tomato blight was obtained with aq. compns. contg. 300 ppm. by wt. of III, IV, V, VI, or

VII. Compns. contg. 500 ppm. by wt. of VI gave excellent control and kill of Aspergillus terreus, Pullularia pullulans, and Rhizopus nigricans.

IT **4726-08-3**, Carbanilic acid, 2,4,6-tribromo-, 2-mercaptoethyl ester, butanesulfonate **4726-12-9**, Methanesulfonic acid, thio-, S-2-hydroxyethyl ester, carbanilate **5017-73-2**, Methanesulfonic acid, thio-, S-3-hydroxypropyl ester, carbanilate
(prepn. of)

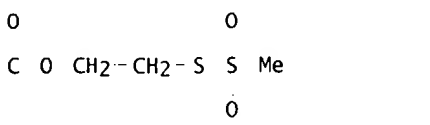
RN 4726-08-3 CAPLUS

CN 1-Butanesulfonothioic acid, S-[2-[[[(2,4,6-tribromophenyl)amino]carbonyl]oxy]ethyl] ester (9CI) (CA INDEX NAME)



RN 4726-12-9 CAPLUS

CN Methanesulfonic acid, thio-, S-(2-hydroxyethyl) ester carbanilate (7CI, 8CI) (CA INDEX NAME)



RN 5017-73-2 CAPLUS

CN Methanesulfonic acid, thio-, S-(3-hydroxypropyl) ester carbanilate (7CI, 8CI) (CA INDEX NAME)